NEWS LOGIN

NEWS IPC8

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Welcome Banner and News Items

For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

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FILE 'HOME' ENTERED AT 15:42:32 ON 08 JAN 2008

=> ile registry

ILE IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> file registry
COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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STRUCTURE FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1 DICTIONARY FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

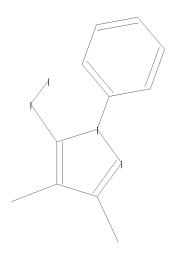
Please note that search-term pricing does apply when conducting SmartSELECT searches.

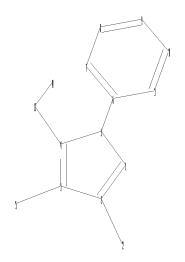
REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

=>

Uploading C:\Program Files\STNEXP\Queries\10581255e.str



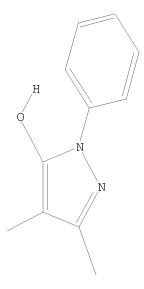


chain nodes :
12 13 14 15
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
2-12 3-15 4-13 5-6 13-14
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 4-13 5-6
exact bonds :
2-12 3-15 13-14
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

=> D L1 L1 HAS NO ANSWERS L1 STR



Structure attributes must be viewed using STN Express query preparation.

=> S L1 fam full

FULL SEARCH INITIATED 15:43:52 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 4156 TO ITERATE

100.0% PROCESSED 4156 ITERATIONS 1 ANSWERS

SEARCH TIME: 00.00.01

L2 1 SEA FAM FUL L1

=> D L2

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN

RN 370557-61-2 REGISTRY

ED Entered STN: 17 Nov 2001

CN 1H-Pyrazol-5-ol, 3,4-dimethyl-1-phenyl- (CA INDEX NAME)

MF C11 H12 N2 O

SR CA

LC STN Files: CA, CAPLUS

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> file caplus
COST IN U.S. DOLLARS

FULL ESTIMATED COST

SINCE FILE TOTAL ENTRY SESSION 72.57 72.78

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008
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FILE COVERS 1907 - 8 Jan 2008 VOL 148 ISS 2 FILE LAST UPDATED: 7 Jan 2008 (20080107/ED)

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/infopolicy.html

=> s L2

L3 1 L2

=> D L3 ibib abs kwic

L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:591008 CAPLUS

DOCUMENT NUMBER: 135:331163

TITLE: Tautomerism in 4-substituted 1-phenyl-3-methyl-

pyrazolin-5-ones-a theoretical ab initio and 13C NMR

study

AUTHOR(S): Kleinpeter, E.; Koch, A.

CORPORATE SOURCE: Institut fur Organische Chemie und Strukturanalytik,

Universitat Potsdam, Potsdam, D-14415, Germany

SOURCE: Journal of Physical Organic Chemistry (2001), 14(8),

566-576

CODEN: JPOCEE; ISSN: 0894-3230

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

AB The tautomeric equilibrium between the CH, OH and NH forms in a series of 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones have been studied using ab initio calcns. at various levels of theory and comparison made with the exptl. results obtained from NMR measurements. Quant. comparison of both the relative energies and the 13C chemical shifts of the tautomers constituting the tautomeric equilibrium were made by calcn. of both sets of parameters. The influence of the solvent was included by employing various models of the self-consistent reaction field theory. Initially, the solvent was included in the calcns. by applying a continuum of differing polarity over the surface of isolated tautomers (self-consistent isodensity polarized continuum model method), then later by assuming formation of an adduct between the solute and the solvent (thereby

simulating effectively the hydrogen bonding in the OH and NH tautomers) and finally by calculating dimer or trimer complexes of the various tautomers. In this manner, the agreement between the theor. calculated and the exptl. determined tautomeric equilibrium was improved significantly. The theor. calculated 13C

chemical shifts of the tautomers were found to be viable for the assignment of the tautomers, particularly the preferred tautomer in the OH/NH equilibrium, which remains fast on the NMR time scale even at low temps.

REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

89-25-8, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl-942-32-5, 1H-Pyrazol-5-ol,3-methyl-1-phenyl- 2721-84-8 4173-74-4, 3H-Pyrazol-3-one, 4-acetyl-2,4-dihydro-5-methyl-2-phenyl-7713-77-1, 3H-Pyrazol-3-one, 1,2-dihydro-4,5-dimethyl-2-phenyl-17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-19735-89-8, 3H-Pyrazol-3-one, 1,2-dihydro-5-methyl-2-phenyl- 27852-31-9 37703-59-6 40864-30-0, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2phenyl- 41927-23-5, 3H-Pyrazol-3-one, 4-bromo-2,4-dihydro-5-methyl-2phenyl-52944-72-6 56634-79-8 64598-47-6 68719-56-2, 3H-Pyrazol-3-one, 4-bromo-1,2-dihydro-5-methyl-2-phenyl-78575-98-1, 1H-Pyrazol-5-ol, 4-bromo-3-methyl-1-phenyl- 78575-99-2, 1H-Pyrazol-5-ol, 3-methyl-4-nitro-1-phenyl- 78576-03-1 138740-34-8 370557-61-2 RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones)

=> file registry COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION FULL ESTIMATED COST 6.15 78.93 DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL ENTRY SESSION CA SUBSCRIBER PRICE -0.80-0.80

FILE 'REGISTRY' ENTERED AT 15:47:41 ON 08 JAN 2008
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STRUCTURE FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1 DICTIONARY FILE UPDATES: 7 JAN 2008 HIGHEST RN 960112-28-1

New CAS Information Use Policies, enter HELP USAGETERMS for details.

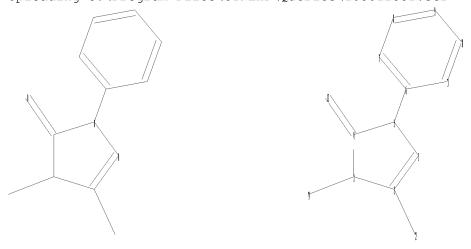
TSCA INFORMATION NOW CURRENT THROUGH June 29, 2007

Please note that search-term pricing does apply when conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html

Uploading C:\Program Files\STNEXP\Queries\10581255f.str

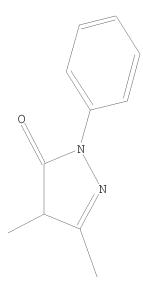


chain nodes :
12 13 14
ring nodes :
1 2 3 4 5 6 7 8 9 10 11
chain bonds :
2-12 3-14 4-13 5-6
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-11 7-8 8-9 9-10 10-11
exact/norm bonds :
1-2 1-5 2-3 3-4 4-13 4-5 5-6
exact bonds :
2-12 3-14
normalized bonds :
6-7 6-11 7-8 8-9 9-10 10-11

Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:CLASS 13:CLASS 14:CLASS

L4 STRUCTURE UPLOADED

=> D L4 L4 HAS NO ANSWERS L4 STR



Structure attributes must be viewed using STN Express query preparation.

=> s L4 fam full FULL SEARCH INITIATED 15:48:28 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 4156 TO ITERATE

100.0% PROCESSED 4156 ITERATIONS 2 ANSWERS SEARCH TIME: 00.00.01

L5 2 SEA FAM FUL L4

=> D L5

L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN

RN 152968-73-5 REGISTRY

ED Entered STN: 11 Feb 1994

CN Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2-phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-, mixt. contg. (9CI)

MF C11 H12 N2 O . C5 H9 N O3

CI MXS

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 17900-68-4 CMF C11 H12 N2 O

CM 2

CRN 106-60-5 CMF C5 H9 N O3

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

=> 1-2

1-2 IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system. For a list of commands available to you in the current file, enter "HELP COMMANDS" at an arrow prompt (=>).

=> D L5 1-2

L5 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN

RN 152968-73-5 REGISTRY

ED Entered STN: 11 Feb 1994

CN Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2-phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-, mixt. contg. (9CI)

MF C11 H12 N2 O . C5 H9 N O3

CI MXS

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

CM 1

CRN 17900-68-4 CMF C11 H12 N2 O

CM 2

CRN 106-60-5 CMF C5 H9 N O3

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L5 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2008 ACS on STN

RN 17900-68-4 REGISTRY

ED Entered STN: 16 Nov 1984

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Pyrazolin-5-one, 3,4-dimethyl-1-phenyl- (6CI, 7CI, 8CI)

OTHER NAMES:

CN 1-Phenyl-3, 4-dimethylpyrazolin-5-one

CN 3,4-Dimethyl-1-phenyl-2-pyrazolin-5-one

CN 3,4-Dimethyl-1-phenylpyrazolone

MF C11 H12 N2 O

CI COM

LC STN Files: BEILSTEIN*, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST,

IFICDB, IFIPAT, IFIUDB, MSDS-OHS, TOXCENTER, USPATFULL, USPATOLD

(*File contains numerically searchable property data)

Other Sources: EINECS**

(**Enter CHEMLIST File for up-to-date regulatory information)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

38 REFERENCES IN FILE CA (1907 TO DATE)

38 REFERENCES IN FILE CAPLUS (1907 TO DATE)

3 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

=> file caplus

COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 76.57 155.50

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE TOTAL
ENTRY SESSION

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -0.80

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http://www.cas.org/infopolicy.html

=> d his

(FILE 'HOME' ENTERED AT 15:42:32 ON 08 JAN 2008)

FILE 'REGISTRY' ENTERED AT 15:42:46 ON 08 JAN 2008

L1 STRUCTURE UPLOADED

L2 1 S L1 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008

L3 1 S L2

FILE 'REGISTRY' ENTERED AT 15:47:41 ON 08 JAN 2008

L4 STRUCTURE UPLOADED

L5 2 S L4 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:49:00 ON 08 JAN 2008

=> s L5

L6 39 L5

=> S L6 and (py<2003 or ay <2003 or pry<2003)

22927520 PY<2003 4474522 AY <2003 3949553 PRY<2003

L7 36 L6 AND (PY<2003 OR AY <2003 OR PRY<2003)

=> D L7 1-10 ibib abs kwic hitstr

L7 ANSWER 1 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:921440 CAPLUS

DOCUMENT NUMBER: 139:391385

TITLE: Pyrazolone analogs for repairing tissue fibrosis INVENTOR(S): Chiba, Akira; Matsumoto, Hideki; Tanaka, Yasuhiro; Ijichi, Chiori; Oomuta, Naoko; Takatsuki, Fumihiko

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 10 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003335672	A	20031125	JP 2002-144720	20020520 <
PRIORITY APPLN. INFO.:			JP 2002-144720	20020520 <
OTHER SOURCE(S):	MARPAT	139:391385		

GΙ

Pyrazolone analogs (I; R1 = (substituted)phenyl; R2, R3 = H; R4 = low alkyl, alkoxy, etc.) and their pharmaceutically acceptable salts are claimed for repairing tissue fibrosis, including liver fibrosis, lung fibrosis, kidney fibrosis, atherosclerosis, prostate hypertrophy, keloid symptom, myocardial symptom, and collagen disease.

PATENT NO. KIND DATE APPLICATION NO. DATE _____ _____ _____ ____ A 20031125 JP 2002-144720 20020520 <--PI JP 2003335672 PRAI JP 2002-144720 20020520 <--

90-31-3 4845-49-2 6402-09-1 6631-89-6 13024-90-3

RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrazolone analogs for repairing tissue fibrosis)

ΙT 17900-68-4

> RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(pyrazolone analogs for repairing tissue fibrosis)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

ANSWER 2 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2003:757683 CAPLUS

139:261293 DOCUMENT NUMBER:

TITLE: Preventive and/or therapeutic agent for hypoxic

ischemic brain disorder

Ikeda, Tomoaki; Ikenoue, Tsuyomu INVENTOR(S): Mitsubishi Pharma Corporation, Japan PATENT ASSIGNEE(S):

SOURCE: PCT Int. Appl., 29 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT	NO.			KIN	D	DATE			APPL	ICAT	ION I	NO.		D	ATE	
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PRIORITY APPLN. INFO.:
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                                              WO 2003-JP3067
                                                                     20030314
                         MARPAT 139:261293
OTHER SOURCE(S):
     The patent relates to a medicine for use in the prevention of and/or
AB
     treatments for hypoxic ischemic brain disorders, especially ones of newborns
     caused by labor. It contains as an active ingredient a substance selected
     from the group consisting of 3-methyl-1-phenyl-2-pyrazolin-5-one,
     pyralozone derivs. which are analogs thereof, physiol. acceptable salts
     thereof, and any hydrates and any solvates of these. Thus,
     1-phenyl-3-methyl-2-pyrazolin-5-one prepared by refluxing Et acetoacetate
     with phenylhydrazine in ethanol and recrystn. was dissolved in simulated
     body fluid and showed effect on hypoxic ischemic brain of new born rat.
     PATENT NO.
                         KIND
                                 DATE
                                            APPLICATION NO.
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                                 _____
                                             _____
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
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     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pyrazolinone derivative for preventive and/or therapeutic agent for
        hypoxic ischemic brain disorder)
ΙT
     17900-68-4
     RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
     (Biological study); USES (Uses)
        (pyrazolinone derivative for preventive and/or therapeutic agent for
        hypoxic ischemic brain disorder)
RN
     17900-68-4 CAPLUS
CN
     3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)
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REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 3 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:591008 CAPLUS

DOCUMENT NUMBER: 135:331163

TITLE: Tautomerism in 4-substituted 1-phenyl-3-methyl-

pyrazolin-5-ones-a theoretical ab initio and 13C NMR

study

AUTHOR(S): Kleinpeter, E.; Koch, A.

CORPORATE SOURCE: Institut fur Organische Chemie und Strukturanalytik,

Universitat Potsdam, Potsdam, D-14415, Germany

SOURCE: Journal of Physical Organic Chemistry (2001

), 14(8), 566-576

CODEN: JPOCEE; ISSN: 0894-3230

PUBLISHER: John Wiley & Sons Ltd.

DOCUMENT TYPE: Journal LANGUAGE: English

The tautomeric equilibrium between the CH, OH and NH forms in a series of 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones have been studied using ab initio calcns. at various levels of theory and comparison made with the exptl. results obtained from NMR measurements. Quant. comparison of both the relative energies and the 13C chemical shifts of the tautomers constituting the tautomeric equilibrium were made by calcn. of both sets of parameters. The influence of the solvent was included by employing various models of the self-consistent reaction field theory. Initially, the solvent was included in the calcns. by applying a continuum of differing polarity over the surface of isolated tautomers (self-consistent isodensity polarized continuum model method), then later by assuming formation of an adduct between the solute and the solvent (thereby simulating effectively the hydrogen bonding in the OH and NH tautomers) and finally by calculating dimer or trimer complexes of the various tautomers. In this manner, the agreement between the theor. calculated and the exptl. determined tautomeric equilibrium was improved significantly. The theor.

calculated 13C

chemical shifts of the tautomers were found to be viable for the assignment of the tautomers, particularly the preferred tautomer in the OH/NH equilibrium, which remains fast on the NMR time scale even at low temps.

SO Journal of Physical Organic Chemistry (2001), 14(8), 566-576 CODEN: JPOCEE; ISSN: 0894-3230

ΙT 89-25-8, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-2-phenyl-942 - 32 - 51H-Pyrazol-5-ol,3-methyl-1-phenyl- 2721-84-8 4173-74-4, 3H-Pyrazol-3-one, 4-acetyl-2,4-dihydro-5-methyl-2-phenyl- 6077-03-8 7713-77-1, 3H-Pyrazol-3-one, 1,2-dihydro-4,5-dimethyl-2-phenyl-17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-19735-89-8, 3H-Pyrazol-3-one, 1,2-dihydro-5-methyl-2-phenyl- 27852-31-9 37703-59-6 40864-30-0, 3H-Pyrazol-3-one, 2,4-dihydro-5-methyl-4-nitro-2phenyl-41927-23-5, 3H-Pyrazol-3-one, 4-bromo-2,4-dihydro-5-methyl-2-68719-56-2, 52944-72-6 56634-79-8 64598-47-6 phenyl-3H-Pyrazol-3-one, 4-bromo-1,2-dihydro-5-methyl-2-phenyl-78575-98-1, 1H-Pyrazol-5-ol, 4-bromo-3-methyl-1-phenyl- 78575-99-2, 1H-Pyrazol-5-ol, 3-methyl-4-nitro-1-phenyl- 78576-03-1 138740-34-8

370557-61-2

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones)

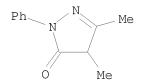
IT 17900-68-4, 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl-

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ab initio and 13C NMR study of tautomerism in 4-substituted 1-phenyl-3-methyl-pyrazolin-5-ones)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)



REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 4 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2001:361602 CAPLUS

DOCUMENT NUMBER: 135:152747

TITLE: Solid-phase synthesis of substituted pyrazolones from

polymer-bound β -keto esters

AUTHOR(S): Tietze, Lutz F.; Evers, Holger; Hippe, Thomas;

Steinmetz, Adrian; Topken, Enno

CORPORATE SOURCE: Institut fur Organische Chemie der

Georg-August-Universitat Gottingen, Gottingen, 37077,

Germany

SOURCE: European Journal of Organic Chemistry (2001

), (9), 1631-1634

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:152747

AB Polymer-bound acetoacetate was γ -mono- and γ -dialkylated, as well as α -monoalkylated. Treatment with hydrazine or substituted hydrazines followed by thermal or acidic cyclizing cleavage yielded the pyrazolones in a purity of >90%.

SO European Journal of Organic Chemistry (2001), (9), 1631-1634 CODEN: EJOCFK; ISSN: 1434-193X

IT 6402-09-1P 7058-21-1P 13051-47-3P 17900-68-4P 22717-41-5P 24246-08-0P 24246-11-5P 26502-95-4P 26645-09-0P 28844-37-3P 40339-61-5P 55294-29-6P 64123-72-4P 76552-51-7P 90688-89-4P 94575-26-5P 118031-38-2P 118049-09-5P 181185-05-7P 181185-06-8P 181185-07-9P 181185-08-0P 181185-09-1P 192209-24-8P 192209-25-9P 192209-26-0P 192209-27-1P 192209-28-2P 352434-76-5P 352434-77-6P RL: SPN (Synthetic preparation); PREP (Preparation)

(solid-phase synthesis of substituted pyrazolones from polymer-bound $\beta\textsc{-keto}$ esters)

IT 17900-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (solid-phase synthesis of substituted pyrazolones from polymer-bound β -keto esters)

RN 17900-68-4 CAPLUS

CN

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 5 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1997:390186 CAPLUS

DOCUMENT NUMBER: 127:95230

TITLE: Solid-phase synthesis of polymer-bound β -keto

esters and their application in the synthesis of

structurally diverse pyrazolones

AUTHOR(S): Tietze, Lutz F.; Steinmetz, Adrian; Balkenhohl,

Friedhelm

CORPORATE SOURCE: Inst. Org. Chem., Georg-August-Univ. Gottingen,

Gottingen, D-37077, Germany

SOURCE: Bioorganic & Medicinal Chemistry Letters (1997

), 7(10), 1303-1306

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Polymer-bound esters of HO2CCHR2COR1 [R1 = CH2Ph, CH2CH2CO2Me, (CH2)3Cl, cyclohexyl, Me; R2 = Me, Et, allyl, CH2CH:CMe2, hexyl,CH2CO2Et] were prepared by treating R1COCl with Meldrum's acid, treating the adduct with polymer-bound ethylene glycol, and alkylating the polymer-bound esters. Mild acid catalyzed reaction with phenylhydrazine or hydrazine occurred with cleavage from the resin and cyclization to give pyrazolones in high purity and good yield.

SO Bioorganic & Medicinal Chemistry Letters (1997), 7(10), 1303-1306

CODEN: BMCLE8; ISSN: 0960-894X

IT 17900-68-4P 22717-41-5P 24246-08-0P 24246-11-5P

26502-95-4P 26645-09-0P 28844-37-3P 90688-89-4P 192209-24-8P

192209-25-9P 192209-26-0P 192209-27-1P 192209-28-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polymer-bound β -keto esters and their conversion to pyrazolones)

IT 17900-68-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of polymer-bound β -keto esters and their conversion to pyrazolones)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

Ph N Me

REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L7 ANSWER 6 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1996:659311 CAPLUS

DOCUMENT NUMBER: 125:300995

TITLE: Preparation of 2-pyrazoline derivatives as herbicides INVENTOR(S): Araino, Nobuyuki; Miura, Juzo; Oda, Yoshiki; Nishioka,

Hitoshi

PATENT ASSIGNEE(S): Nihon Nohyaku Co Ltd, Japan SOURCE: Jpn. Kokai Tokkyo Koho, 63 pp.

CODEN: JKXXAF

Ι

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08217777 PRIORITY APPLN. INFO.:	A	19960827	JP 1995-46427 JP 1995-46427	19950210 < 19950210 <
OTHER SOURCE(S): GI	MARPAT	125:300995		

$$\begin{array}{c|c}
 & CH_2 - C \\
 & R_1 & R_2 \\
 & R_2 & R_2
\end{array}$$

AB The title compds. [I; R = (un)substituted alkyl or alkenyl or Ph or pyridinyl, etc.; R1, R2 = H, (un)substituted alkyl or alkenyl, etc.; X = halo, NO2, (un)substituted alkyl or amino, etc.; n = 0-5; Z = CH2O] and their intermediates (Z = O, :CH2; others are same as above) are claimed. Herbicides containing I are effective against Amaranthus lividus, Scirpus juncoides, and Monochoria vaginalis. Thus, trimethylsulfonium iodide was treated with NaH and then reacted with 4-benzoylmethyl-4-ethyl-3-methyl-1-phenyl-2-pyrazolin-5-one to give 55% a mixture of diastereoisomers I (R = Ph, R1 = Et, R2 = Me, X = H, n = 5, Z = CH2O) (II). Herbicides containing II at 3 kg/ha preemergence showed 100% herbicidal effect for Amaranthus lividus and Scirpus juncoides.

PI JP 08217777 A 19960827 Heisei

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
 JP 08217777 JP 1995-46427	A	19960827 19950210 <	JP 1995-46427 <	19950210 <

IT 106-95-6, Allyl bromide, reactions 2181-42-2, Trimethylsulfonium iodide 7534-40-9 17900-68-4 41011-01-2, 3-Chlorophenacyl bromide <math>182875-62-3

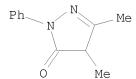
RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pyrazoline derivs. as herbicides)

IT 17900-68-4

RL: RCT (Reactant); RACT (Reactant or reagent) (preparation of pyrazoline derivs. as herbicides)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)



L7 ANSWER 7 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1995:133733 CAPLUS

DOCUMENT NUMBER: 123:142959

TITLE: Steering effects of phase transfer catalysts on the

benzylation of 2-naphtholate and the methylation of

3-methyl-1-phenyl-5-pyrazolone

AUTHOR(S): Dehmlow, Eckehard V.; Klauck, Robert

CORPORATE SOURCE: Fakultat Chemie, Univ. Bielefeld, Bielefeld, D-33615,

Germany

SOURCE: Journal of Chemical Research, Synopses (1994

), (11), 448-9

CODEN: JRPSDC; ISSN: 0308-2342

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 123:142959

AB O- vs. C-alkylation and bis-alkylation of 2-naphthol and O-, N- and C-alkylation or bis-alkylation of 3-methyl-1-phenyl-5-pyrazolone can be influenced by the nature and the presence of the phase transfer (PT) catalyst.

Journal of Chemical Research, Synopses (1994), (11), 448-9 CODEN: JRPSDC; ISSN: 0308-2342

IT 17900-68-4

SO

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(chemoselectivity by phase transfer catalysts in methylation of 3-methyl-1-phenyl-5-pyrazolone)

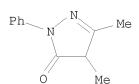
IT 17900-68-4

RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)

(chemoselectivity by phase transfer catalysts in methylation of 3-methyl-1-phenyl-5-pyrazolone)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)



L7 ANSWER 8 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1994:127807 CAPLUS

DOCUMENT NUMBER: 120:127807

TITLE: Herbicidal δ -aminolevulinic acid combinations

with chlorophyll biosynthesis modulators.

INVENTOR(S): Rebeiz, Constantin A.

PATENT ASSIGNEE(S): Board of Trustees of the University of Illinois, USA

U.S., 40 pp. Cont.-in-part of U.S. 5,163,990. SOURCE:

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PA	IENT NO.		KIND	DATE	APPLICATION NO.	
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US	5163990		A	19921117	US 1990-521119	19900503 <
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AB The	e title compr	ıs. a	re defo	liants an	d herbicides, with ac	

the accumulation of photodynamic tetrapyrrols. A mixture of 20 mM γ -aminolevulinic acid and 15 mM 6-aminonicotinic acid defoliated tomato seedlings.

	S 5242892 A ATENT NO.	19930907 KIND	DATE	APPLICATION NO.	DATE
EF	5 5242892 2 331211 2 331211	A A2 A3	19930907 19890906 19891123	US 1990-615413 EP 1989-106579	19901119 < 19850717 <
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                                            152968-94-0
                                                         152968-95-1
    152968-96-2
                 152968-97-3
                               152968-98-4
                                            152968-99-5
                                                         152969-00-1
                 152969-02-3 153145-67-6
    152969-01-2
    RL: AGR (Agricultural use); BAC (Biological activity or effector, except
    adverse); BSU (Biological study, unclassified); BIOL (Biological study);
```

USES (Uses)

(herbicide and defoliant)

ΙT 152968-73-5

> RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study); USES (Uses)

(herbicide and defoliant)

RN 152968-73-5 CAPLUS

Pentanoic acid, 5-amino-4-oxo-, mixt. with 2,4-dihydro-4,5-dimethyl-2-CN phenyl-3H-pyrazol-3-one (9CI) (CA INDEX NAME)

CM 1

CRN 17900-68-4 CMF C11 H12 N2 O

CM

CRN 106-60-5 CMF C5 H9 N O3

$$\begin{array}{c} {\rm O} \\ || \\ {\rm H_2N-CH_2-C-CH_2-CH_2-CO_2H} \end{array}$$

ANSWER 9 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1993:223017 CAPLUS

DOCUMENT NUMBER: 118:223017

TITLE: Nonsubstantive color developer for color filter and

its use in manufacturing color filter for color

liquid crystal display

Shimizu, Hiroshi; Miyaoka, Kazuyoshi; Hirota, Kenji; INVENTOR(S):

Koboshi, Shigeharu

PATENT ASSIGNEE(S):

Konica Co., Japan Jpn. Kokai Tokkyo Koho, 16 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04009053	A	19920113	JP 1990-109583	19900425 <
PRIORITY APPLN. INFO.:			JP 1990-109583	19900425 <
GI				

 ${\tt AB}$ A nonsubstantive color developer for a color filter contains a high concentration

of Br- ion and ≥ 1 bias coupler [I; R = (un)substituted alkyl or aryl substituted at the active site; X = atoms required to form an(un)substituted (ring-fused) 5- or 6-membered ring containing ≥ 1 N, S, or O; the heterocyclic ring or the alkyl group is substituted with a C2-24 organic group which allows I to completely or partially dissolve in a processing solution and after coupling with the oxidized color developing agent, imparts I a mol. size and shape nondiffusible in an emulsion layer]. The Br- concentration is preferably ≥ 0.05 mol/L. A color filter is manufactured by (1) pattern-wise exposure of a photosensitive material having a Ag halide emulsion layer containing Ag halide micrograins formed on a transparent substrate and (2) nonsubstantive development by the above nonsubstantive color developer to form dye images corresponding to the patterns. The process reduces relief between pixels with different spectral characteristics, thus gives excellent surface smoothness, prevents fog in the unexposed parts, and gives sufficient d. in the exposed parts.

PI JP 04009053 A 19920113 Heisei

PATENT NO. KIND DATE APPLICATION NO. DATE

PI JP 04009053 A 19920113 JP 1990-109583 19900425 <--

PRAI JP 1990-109583 19900425 <--

IT 17900-68-4 125740-63-8 131443-12-4 147163-78-8

RL: USES (Uses)

(bias coupler, nonsubstantive color developer containing bromide ions and, for color filter)

IT 17900-68-4

RL: USES (Uses)

(bias coupler, nonsubstantive color developer containing bromide ions and, for color filter)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

L7 ANSWER 10 OF 36 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 1991:52993 CAPLUS

DOCUMENT NUMBER: 114:52993

TITLE: Color filter for liquid-crystal color display device INVENTOR(S): Mochizuki, Yoshiharu; Okauchi, Ken; Masukawa, Toyoaki

PATENT ASSIGNEE(S): Konica Co., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02191903	A	19900727	JP 1989-79302	19890329 <
PRIORITY APPLN. INFO.:			JP 1988-241800	A1 19880927 <
	_	613.		

AB A process for making a color filter for a liquid-crystal color display device comprises forming color images from a patternwise exposed Ag halide emulsion layer on a transparent support, using a developer solution containing couplers and color developing agents, wherein the images are treated with a processing solution containing a coupler capable of forming a substantially colorless compound by reacting with the oxidized color developing agent and having a pH ≥ 9 at 25° .

PI JP 02191903 A 19900727 Heisei

	0	1000101				
	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
ΡI	JP 02191903	A	19900727	JP 1989-79302	19890329	<
PRAI	JP 1988-241800	A1	19880927	<		
TТ	17900-68-4 72	705-83-0	119105-62-	3 131443-12-4	131443-13-5	

IT 17900-68-4 72705-83-0 119105-62-3 131443-12-4 131443-13-5 131443-14-6 131443-15-7 131443-16-8 131443-17-9 131443-18-0 RL: USES (Uses)

(photog. processing solns. containing, for fabrication of color filters for liquid-crystal display devices)

IT 17900-68-4

RL: USES (Uses)

(photog. processing solns. containing, for fabrication of color filters for liquid-crystal display devices)

RN 17900-68-4 CAPLUS

CN 3H-Pyrazol-3-one, 2,4-dihydro-4,5-dimethyl-2-phenyl- (CA INDEX NAME)

=> D his

(FILE 'HOME' ENTERED AT 15:42:32 ON 08 JAN 2008)

FILE 'REGISTRY' ENTERED AT 15:42:46 ON 08 JAN 2008

L1 STRUCTURE UPLOADED

L2 1 S L1 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:44:08 ON 08 JAN 2008

L3 1 S L2

FILE 'REGISTRY' ENTERED AT 15:47:41 ON 08 JAN 2008

L4 STRUCTURE UPLOADED

L5 2 S L4 FAM FULL

FILE 'CAPLUS' ENTERED AT 15:49:00 ON 08 JAN 2008

L6 39 S L5

L7 36 S L6 AND (PY<2003 OR AY <2003 OR PRY<2003)

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